Supporting Information

Adsorption and sensor performance of transition metals decorated zirconium-doped silicon carbide nanotubes for NO_2 gas application: A computational insight

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Table S1. Result of the molecular dynamic simulations for the surfaces before interactions.

Parameters	Initial	Final	Average ± Std. Dev
Zr@SiCNT			
Tot. energy (kcal/mol)	83.032	83.200	83.263 ± 0.043
Pot. energy (kcal/mol)	-4.019	40.205	39.957 ± 2.629
Kin. energy (kcal/mol)	87.051	42.995	43.305 ± 2.611
Temperature (K)	298.000	147.183	148.246 ± 8.940
Ag_Zr@SiCNT			
Tot. energy (kcal/mol)	105.906	106.307	106.288 ± 0.049
Pot. energy (kcal/mol)	17.967	61.647	60.202 ± 2.863
Kin. energy (kcal/mol)	87.940	44.660	46.086 ± 2.844
Temperature (K)	298.000	151.340	156.171 ± 9.639
Au_Zr@SiCNT			
Tot. energy (kcal/mol)	93.492	93.841	93.832 ± 0.059
Pot. energy (kcal/mol)	5.552	50.782	48.762 ± 2.815
Kin. energy (kcal/mol)	87.940	43.059	45.070 ± 2.786
Temperature (K)	298.000	145.912	152.729 ± 9.441
Cu_Zr@SiCNT			
Tot. energy (kcal/mol)	196.393	196.763	196.758 ± 0.046
Pot. energy (kcal/mol)	108.453	151.229	148.579 ± 3.039
Kin. energy (kcal/mol)	87.940	45.534	48.179 ± 3.019
Temperature (K)	298.000	154.300	163.262 ± 10.229

Parameters	Initial	Final	Average ± Std. Dev
NO_2_n_Zr@SiCNT			
Tot. energy (kcal/mol)	288.863	289.248	289.270 ± 0.045
Pot. energy (kcal/mol)	199.146	241.591	244.539 ± 2.641
Kin. energy (kcal/mol)	89.716	47.656	44.731 ± 2.620
Temperature (K)	298.000	158.294	148.577 ± 8.703
NO_2_n_Ag_Zr@SiCNT			
Tot. energy (kcal/mol)	361.520	361.790	361.871 ± 0.048
Pot. energy (kcal/mol)	270.915	316.830	313.882 ± 2.845
Kin. energy (kcal/mol)	90.605	44.959	47.990 ± 2.824
Temperature (K)	298.000	147.872	157.838 ± 9.287
NO_2_n_Au_Zr@SiCNT			
Tot. energy (kcal/mol)	222.790	222.956	223.068 ± 0.036
Pot. energy (kcal/mol)	132.186	163.826	170.142 ± 3.335
Kin. energy (kcal/mol)	90.605	59.131	52.926 ± 3.318
Temperature (K)	298.000	194.483	174.076 ± 10.914
NO_2_n_Cu_Zr@SiCNT			
Tot. energy (kcal/mol)	187.956	188.283	188.265 ± 0.042
Pot. energy (kcal/mol)	97.351	143.941	143.052 ± 2.702
Kin. energy (kcal/mol)	90.605	44.342	45.213 ± 2.682
Temperature (K)	298.000	145.840	148.706 ± 8.821

Table S2. Result of the molecular dynamic simulations for the resulting complexes due to the n-site of adsorption

Parameters	Initial	Final	Average ± Std. Dev
NO_2_o_Zr@SiCNT			
Tot. energy (kcal/mol)	146.233	146.601	146.562 ± 0.038

Table S3. Result of the molecular dynamic simulations for the resulting complexes due to the o-site of adsorption

Pot. energy (kcal/mol)	56.516	102.623	101.859 ± 2.633
Kin. energy (kcal/mol)	89.716	43.978	44.702 ± 2.617
Temperature (K)	298.000	146.078	148.483 ± 8.694
NO_2_o_Ag_Zr@SiCNT			
Tot. energy (kcal/mol)	305.996	306.517	306.427 ± 0.077
Pot. energy (kcal/mol)	215.391	264.480	261.080 ± 2.683
Kin. energy (kcal/mol)	90.605	42.037	45.348 ± 2.645
Temperature (K)	298.000	138.261	149.149± 8.700
NO_2_o_Au_Zr@SiCNT			
Tot. energy (kcal/mol)	213.363	213.858	213.841 ± 0.092
Pot. energy (kcal/mol)	122.758	163.526	161.273 ± 3.945
Kin. energy (kcal/mol)	90.605	50.332	52.569 ± 3.908
Temperature (K)	298.000	165.543	172.899 ± 12.854
NO_2_o_Cu_Zr@SiCNT			
Tot. energy (kcal/mol)	329.161	329.525	329.521 ± 0.067
Pot. energy (kcal/mol)	238.556	280.427	279.460 ± 3.098
Kin. energy (kcal/mol)	90.605	49.098	50.060 ± 3.069
Temperature (K)	298.000	161.485	164.650 ± 10.094